Modern Quantum Mechanics.

Chapter I. Fundamental Concepts

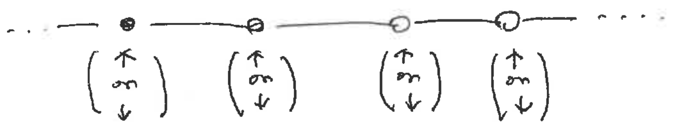
1.1 Hilbert space and state vector

Hilbert space $\xleftarrow{\text{a generalization}}$ Euclidean Space (2D. 3D)

→ can have $\left(\begin{matrix}\text{any finite} \\ \text{infinite}\end{matrix}\right)$ dim. !

• Hilbert space dimension in QM : examples.

⇒ spin-$\frac{1}{2}$ chain



Q. How many "states" are available ? (accessible)

# of possible configurations

$= 2^N$ ← dim. of H-space.

⇒ a free particle

"•" (It's just flying in any direction)

↑ "position" : can be anything !

→ H-space dimension : infinite !

cf. what about "momentum" ?

It's conserved.

→ H-space is just a point if $\vec{p}$ is known.

(reduced into)

- What does "a generalization" mean?

- H-space : a vector space.

  ↳ works just like in 2D or 3D Euclidean space.

- In 3D E-space.

$$\vec{x} \doteq \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \underbrace{x \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} + y \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} + z \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}}_{\text{"basis"}}$$

→ inner products are well-defined!

→ length, angle.

- In H-space.

  - ex. spin-$\frac{1}{2}$ chain

state vector

$$\Psi \doteq a_1 (\uparrow \downarrow \uparrow \cdots) + a_2 (\downarrow \downarrow \uparrow \cdots) + a_3 (\downarrow \uparrow \downarrow \cdots) \\ \vdots$$

many terms.

$a_1, a_2, \cdots$: complex in gen.

But, it's a linear combination!

and, the inner products are also defined! ←

$(\uparrow \downarrow \uparrow) \perp (\downarrow \downarrow \uparrow)$

No overlaps! : "orthogonal"

- Math. formulation of a "state vector"

  ↳ Bra-Ket notation (Dirac).

1.2 Kets, Bras, Operators.

- H-space : a complex vector space.

(1) a state vector $\doteq$ a "ket" vector $\boxed{|\alpha\rangle}$

works like a "vector".

- addition : $|\gamma\rangle = |\alpha\rangle + |\beta\rangle$
- addition is commutative : $|\alpha\rangle + |\beta\rangle = |\beta\rangle + |\alpha\rangle$ for all $|\alpha\rangle$ and $|\beta\rangle$.
- there exists a "null" vector $|\emptyset\rangle$.

$$|\alpha\rangle + |\emptyset\rangle = |\emptyset\rangle + |\alpha\rangle = |\alpha\rangle$$

- multiplication by any c-number : $|\alpha'\rangle = c|\alpha\rangle$.
- distributive law : $a(|\alpha\rangle + |\beta\rangle) = a|\alpha\rangle + a|\beta\rangle$

(2) an observable, an operator, an eigenket.

same concept.

" an observable can be represented by an operator."

$$\Rightarrow \quad A|\alpha\rangle = \text{another ket, in general.}$$

an operator

- Eigenket $\doteq$ Eigenvector

"eigen"

the same ket

$$A|a_1\rangle = a_1|a_1\rangle, \quad A|a_2\rangle = a_2|a_2\rangle \quad \cdots\cdots$$

a number. (eigenvalue)

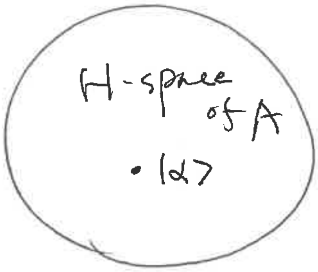
- Eigenstate : a physical state corresponding to an eigenket.

ex. $S_z|S_z;+\rangle = \frac{\hbar}{2}|S_z;+\rangle, \quad S_z|S_z;-\rangle = -\frac{\hbar}{2}|S_z;-\rangle$

$\Rightarrow$ N-dim. H-space of A.

$\uparrow$ spanned by N eigenkets of A. $\{|a'\rangle\}$

$\therefore$ $$|\alpha\rangle = \sum_{a'} c_{a'} |a'\rangle$$



(3) Bra space and Inner Products

: is dual to the ket space

ket vec.

bra vector

$$|\alpha\rangle \longleftrightarrow \langle\alpha|$$

Dual Correspondence

If $|\gamma\rangle = c_\alpha|\alpha\rangle + c_\beta|\beta\rangle$,

$$\xleftrightarrow{\text{D.C.}} \quad c_\alpha^* \langle\alpha| + c_\beta^* \langle\beta|$$

complex conj.

- Inner product : $\langle\beta|\alpha\rangle = (\langle\beta|)\cdot(|\alpha\rangle)$

$\Leftarrow$ a generalization of $x^T \cdot y$

property 1. $\langle\beta|\alpha\rangle = \langle\alpha|\beta\rangle^*$: complex conj.

property 2. $\boxed{\langle\alpha|\alpha\rangle} = \langle\alpha|\alpha\rangle^* \quad \boxed{\geq 0.}$

: positive definite metric unless $|\alpha\rangle = |0\rangle$

- This is essential to the probabilistic interpretation of Q.M.

- $|\alpha\rangle$ and $|\beta\rangle$ are orthogonal if $\langle\alpha|\beta\rangle = 0$.

- normalization : $|\tilde{\alpha}\rangle = \dfrac{1}{\left[\sqrt{\langle\alpha|\alpha\rangle}\right]} |\alpha\rangle$

  ↳ norm of $|\alpha\rangle$

  $\Rightarrow \langle\tilde{\alpha}|\tilde{\alpha}\rangle = 1$

  ~ length of a vector.

(4) Operators.

- equal operators $X = Y$ if $X|\alpha\rangle = Y|\alpha\rangle$ for an arb. ket.

- null operator : $X|\alpha\rangle = 0$.

- Cummulative and associative addition

  $X + Y = Y + X$, $X + (Y + Z) = (X + Y) + Z$

- Linear operator : $X(c_\alpha|\alpha\rangle + c_\beta|\beta\rangle) = c_\alpha X|\alpha\rangle + c_\beta X|\beta\rangle$
  (most ops in Q.M.)

- duality :

  $X|\alpha\rangle \overset{D.C.}{\longleftrightarrow} \langle\alpha|X^+$!

  Hermitian adjoint.

- Hermitian op : $X = X^+$

(5) Multiplication ~ matrix multiplication.

- Noncommutative, in general !

  $XY \neq YX$.

- associative : $X(YZ) = (XY)Z \equiv XYZ$

- $(XY)^+ = Y^+X^+$

  because. $X(Y|\alpha\rangle) \overset{D.C.}{\longleftrightarrow} (\langle\alpha|Y^+)X^+$ $= (XY)^+$

- Outer product of $|\beta\rangle$, $\langle\alpha|$

  : $|\beta\rangle\langle\alpha|$ ← This is also an operator.

  (c.f. $\langle\alpha|\beta\rangle$ = number)

- Illegal products : $X\langle\alpha|$ (×), $|\alpha\rangle X$ (×), $|\alpha\rangle|\beta\rangle$ (×) or $\langle\alpha|\langle\beta|$ (×) (if $|\alpha\rangle, |\beta\rangle$ are in the same H-space) "Nonsense"

(6) Associative Axiom.

- $(|\beta\rangle\langle\alpha|)\cdot|\gamma\rangle = |\beta\rangle\cdot(\underbrace{\langle\alpha|\gamma\rangle}_{\text{number}})$

  means ↳ it rotates $|\gamma\rangle$ into the direction of $|\beta\rangle$.

- $\langle\beta|X|\alpha\rangle = \langle\beta|\cdot(X|\alpha\rangle) = (\langle\beta|X)\cdot|\alpha\rangle$

- Hermitian ⇒ $\langle\beta|X|\alpha\rangle = \langle\alpha|X|\beta\rangle^*$.

  proof.

$$\begin{aligned}\langle\beta|X|\alpha\rangle &= \langle\beta|\cdot(X|\alpha\rangle) \\ &= \left[(\langle\alpha|X^\dagger)\cdot|\beta\rangle\right]^* \\ &= \langle\alpha|X^\dagger|\beta\rangle^* = \langle\alpha|X|\beta\rangle^*\end{aligned}$$

if X is Hermitian

1.3 Base Kets and Matrix representation

(1) Eigenkets of an observable

Theorem. Eigenvalues of a Hermitian op : Real

Eigenvectors corrs. diff. eigenvalues – kets are "orthogonal"!

proof.

Eigenket of A : $\{|a_i\rangle\}$, Eigenvalues : $\{a_i\}$

$\rightarrow$ $A|a_i\rangle = a_i|a_i\rangle$, $\langle a_j|A = a_j^* \langle a_j|$

(A : Hermitian)

Then, $(a_i - a_j^*)\langle a_j|a_i\rangle = 0$ //

① if $a_i = a_j$, $a_i = a_j^*$ // (since $\langle a_i|a_i\rangle \neq 0$).

(eigenvalues are real)

② if $a_i \neq a_j$, $\langle a_j|a_i\rangle = 0$. (since $a_i - a_j^* = a_i - a_j \neq 0$

(orthogonal eigenkets))

Eigenkets are normalized : $\langle a_j|a_i\rangle = \delta_{ij}$ // #

(2) Eigenkets as Base ~~kets~~.

recall : an arbitrary ket $|\alpha\rangle$ in H-space of A .

$\rightarrow$ expansion with the eigenkets of A . ($\{|a\rangle\}$) .

$$|\alpha\rangle = \sum_{a'} C_{a'}|a'\rangle .$$

now, we know C_a by $\langle a| \times$

$C_a = \langle a|\alpha\rangle$. (since $\langle a|a'\rangle = \delta_{aa'}$ (orthogonality)) .

Now, one can rewrite $|\alpha\rangle$ as

$$|\alpha\rangle = \sum_a |a\rangle\langle a|\alpha\rangle = \underbrace{\left[\sum_a |a\rangle\langle a|\right]}_{= I \text{ (identity op)}} \cdot |\alpha\rangle$$

$$\sum_a |a\rangle\langle a| = \mathbb{1}$$: completeness relation (closure)

very important.

ex. $\langle\alpha|\alpha\rangle = 1 \to$ condition for C_a?

$$\langle\alpha|\alpha\rangle = \langle\alpha| \cdot \sum_a |a\rangle\langle a| \cdot |\alpha\rangle$$

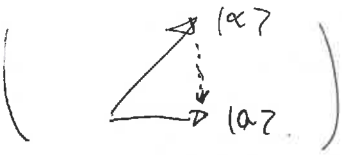
$$= \sum_a |\langle a|\alpha\rangle|^2 = \sum_a |C_a|^2 = 1.$$

Another expression with a projection operator.

- projection operator def. $\boxed{\Lambda_a = |a\rangle\langle a|}$

meaning : $\Lambda_a|\alpha\rangle = \langle a|\alpha\rangle|a\rangle$

$\to$ Λ_a selects the portion of the ket $|\alpha\rangle$ parallel to $|a\rangle$.



Completeness : $\sum_a \Lambda_a = I$

(Summing up all proj.s $\to$ It has to be "complete".)

* for a continuous parameter a,

$$\int da\, |a\rangle\langle a| = 1$$